An efficient numerical algorithm on irreducible multiparty correlations

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We develop a numerical algorithm to calculate the degrees of irreducible multiparty correlations for an arbitrary multiparty quantum state, which is efficient for any quantum state of up to five qubits. We demonstrate the power of the algorithm by the explicit calculations of the degrees of irreducible multiparty correlations in the 4-qubit GHZ state, the Smolin state, and the 5-qubit W state. This development takes a crucial step towards practical applications of irreducible multiparty correlations in real quantum many-body physics.

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Introduction.— In modern physics, as is well known, mean field theory is not sufficient to describe the physics in a strongly correlated many-body system [1], which implies that there exist rich correlation structures in its quantum state. Therefore, how to characterize multiparty correlations in a multipartite quantum state becomes a fundamental problem in many-body physics. Traditional physical method is to introduce the correlation functions to describe the correlations in a many-body system.

The extensive researches on characterizing entanglement in quantum information science [2] shed different light on the problem. On one hand, correlation functions are not invariant under local unitary transformations, which implies that they can be regarded only as correlation witnesses but not as legitimate correlation measures [3, 4]. On the other hand, the information based viewpoint can be instructive in characterizing correlations in a multipartite quantum state.

In the information viewpoint, the degree of the total correlation [5] in a multipartite quantum system is equal to the difference between the sum of von Neumann entropies of all the subsystems and the von Neumann entropy of the whole system. There are two different schemes to classify the total correlation: one is to distinguish the total correlation into quantum correlation and classical correlation [3, 6], the other is to divide the total correlation into pairwise correlation, triplewise correlation, etc..

The concept of irreducible n-party correlation in an n-partite quantum state was first proposed in Ref. [7]. We generalized it to irreducible m-party ($2 \leq m \leq N$) correlation in an n-partite state, and proposed that all the irreducible m-party correlations construct a classification of the total correlation [8, 9]. It is worthy to note that, in classical information community, the irreducible m-party correlations in a joint probability distribution of n classical random variables were investigated in Ref. [10, 11].

The degree of irreducible multiparty correlations in a multipartite quantum state, like many important quantities in quantum information science, such as the measure of entanglement [12] and the capacity of a quantum channel [13, 14], are defined as an optimization problem, which makes their calculations become extremely difficult. These computational difficulties almost prevent any practical application of these measures in a real physical problem. Therefore it is of great significance to develop an efficient algorithm to calculate them for a general multiparty quantum state.

In Ref. [8], we proposed a continuity approach that reduces the calculations of irreducible multiparty correlations in a multiparty quantum state without maximal rank to the calculations of irreducible multiparty correlations in a series of multiparty quantum states with maximal rank. Although theorem 1 in Ref. [8] tells us the form of a maximal rank state without higher order irreducible multiparty correlations, however, this theorem does not solve the problem on the calculations of irreducible multiparty correlations for a general multiparty quantum state with maximal rank. This is why we solve the calculations only for some specific classes of states in Ref. [8]. In other words, we have not a systematic method to calculate the irreducible multiparty correlations for a state with maximal rank.

In this Letter, we develop an efficient systematic numerical algorithm on the calculations of the degrees of irreducible multiparty correlations for a general multipartite quantum state.The advantages of our algorithm is that it is independent of initial values of variables, and we find it is efficient for an arbitrary quantum state of up to five qubits. To the best of our knowledge, it is for the first time that we have the capacity to deal with the detailed analysis of the correlations in a general multiparty state of up to five qubits.

Notations and Definitions.— The Hilbert space of an n-partite quantum system is denoted by $\mathcal{H}^{[n]} \equiv \prod_{i=1}^{n} \otimes \mathcal{H}^{(i)}$, where $[n]$ is the set $\{1, 2, \cdots, n\}$, and $\mathcal{H}^{(i)}$ is the Hilbert space of party i whose dimension is d_i. The inner product of two operators $A^{(i)}$ and $B^{(i)}$ in the Hilbert space $\mathcal{H}^{(i)}$ is defined as $\langle A^{(i)}|B^{(i)}\rangle = \frac{1}{d_i}\mathrm{Tr}(A^{(i)\dagger}B^{(i)})$ [15]. The prefactor $\frac{1}{d_i}$ is introduced to satisfy the normalization condition $\langle I^{(i)}|I^{(i)}\rangle = 1$,

where $I^{(i)}$ is the identity operator in the Hilbert space $\mathcal{H}_i$. Thus we can introduce an orthonormal Hermitian operator basis $\{O_{a_i}^{(i)}, a_i \in \{0,1,\cdots,d_i^2-1\}\}$. In particular, we take $O_0^{(i)}$ to be the identity operator $I^{(i)}$. Any operator $A^{(i)}$ can be expanded in this basis as $A^{(i)} = \sum_{a_i} O_{a_i}^{(i)} \langle O_{a_i}^{(i)}|A^{(i)}\rangle$. Further more, the operator $A^{[n]}$ in the n-party Hilbert space can be expanded as $A^{[n]} = \sum_{\mathbf{a}(n)} O_{\mathbf{a}(n)}^{[n]} \langle O_{\mathbf{a}(n)}^{[n]}|A^{[n]}\rangle$, where $\mathbf{a}(n)$ is the set $\{a_1, a_2, \cdots, a_n\}$, and $O_{\mathbf{a}(n)}^{[n]}$ is an abbreviated notation for $\prod_{i=1}^n O_{a_i}^{(i)}$. If the operator $A^{[n]}$ is the Hamiltonian of an n-party system, the terms to describe m-party interactions ($1 \le m \le n$) satisfy the condition $N_0(\mathbf{a}(n)) = n-m$ with $N_0(\mathbf{a}(n)) = \sum_{a_i} \delta_{0a_i}$.

Without loss of generality, we consider an n-party quantum state $\rho^{[n]}$ with maximal rank, which can be expanded as

$$\rho^{[n]} = \sum_{\mathbf{a}(n)} O_{\mathbf{a}(n)}^{[n]} \langle O_{\mathbf{a}(n)}^{[n]}|\rho^{[n]}\rangle. \tag{1}$$

Because the state $\rho^{[n]}$ is positive definite, we can define $\ln \rho^{[n]}$ uniquely as a Hermitian operator. Then we can apply the above expansion to $\ln \rho^{[n]}$ to obtain

$$\ln \rho^{[n]} = \sum_{\mathbf{a}(n)} O_{\mathbf{a}(n)}^{[n]} \langle O_{\mathbf{a}(n)}^{[n]}|\ln \rho^{[n]}\rangle. \tag{2}$$

The condition $\mathrm{Tr}\rho^{[n]} = 1$ implies that the coefficient $\langle O_{\mathbf{0}(n)}^{[n]}|\ln \rho^{[n]}\rangle$ can be determined by the other coefficients $\langle O_{\tilde{\mathbf{a}}(n)}^{[n]}|\ln \rho^{[n]}\rangle$. Here $\mathbf{0}(n)$ is the set $\mathbf{a}(n)$ with $a_i = 0$ for $i \in [n]$, and $\tilde{\mathbf{a}}(n)$ is the same as $\mathbf{a}(n)$ except $\mathbf{0}(n)$. Compared with the expansion (1), the obvious advantage of the expansion (2) is that it ensures the positivity of $\rho^{[n]}$ automatically. Further more, a one-to-one map between the state $\rho^{[n]}$ with maximal rank and the set of real coefficients $\{\langle O_{\tilde{\mathbf{a}}(n)}^{[n]}|\ln \rho^{[n]}\rangle\}$ can be built. The existence of such a one-to-one map is an essential element in our numerical algorithm.

To make use of the expansion (2), we adopt the equivalent definitions of the degrees of irreducible multiparty correlations in a multiparty quantum state given in Ref. [9] but not the original definitions proposed in Ref. [7, 8]. If we adopt the original definition, then the optimization is made under the expansion (1) , which makes the optimization almost impossible because of the constraint of semipositivity of a density matrix. In Ref. [9], we give the definitions on the degrees of irreducible multiparty correlations for a three-qubit system. Now the definitions are generalized for a general multipartite quantum state with a finite dimensional Hilbert space as follows.

We first define the set of the n-party states without more-than-m-party irreducible correlations as

$$B_m \equiv \{\sigma^{[n]}|\langle O_{\mathbf{a}(n)}^{[n]}|\ln \sigma^{[n]}\rangle = 0, \forall N_0(\mathbf{a}(n)) < n-m\}. \tag{3}$$

Next we find the state in the set B_m that is least distinguishable with the state $\rho^{[n]}$

$$\rho_m^{[n]} \equiv \arg \min_{\sigma^{[n]} \in B_m} S(\rho^{[n]}||\sigma^{[n]}), \tag{4}$$

where the quantum relative entropy [16] $S(\rho||\rho') = \mathrm{Tr}(\rho(\ln \rho - \ln \rho'))$ for two quantum states ρ and ρ' in the same Hilbert space. Then the degree of irreducible m-party correlation is defined as

$$C_m(\rho^{[n]}) \equiv S(\rho_m^{[n]}||\rho_{m-1}^{[n]}). \tag{5}$$

In addition, the degree of the total correlation is defined by

$$C_T(\rho^{[n]}) \equiv S(\rho^{[n]}||\rho_1^{[n]}). \tag{6}$$

Using the same arguments given in Ref. [9], we can show that $C_T(\rho^{[n]}) = \sum_{m=2}^n C_m(\rho^{[n]}) = \sum_{i=1}^n S(\rho^{(i)}) - S(\rho^{[n]})$ with the von Neaumann entropy $S(\rho) = -\mathrm{Tr}(\rho \ln \rho)$ for a quantum state ρ.

Numerical Algorithm.— In the above optimization problem, it is an essential task to find out the state $\rho_m^{[n]}$ for a given state $\rho^{[n]}$. It is possible to directly solve Eq. (4) to obtain the state $\rho_m^{[n]}$. However, it is doutful whether the solution we find is a local minimum or a global minimum. Fortunately, the optimization problem (4) can be transformed into the following system of nonlinear equations:

$$\langle O_{\mathbf{a}(n)}^{[n]}|\ln \rho_m^{[n]}\rangle = 0, \quad \forall N_0(\mathbf{a}(n)) < n-m, \tag{7}$$

$$\langle O_{\mathbf{a}(n)}^{[n]}|\rho_m^{[n]}\rangle = \langle O_{\mathbf{a}(n)}^{[n]}|\rho^{[n]}\rangle, \quad \forall N_0(\mathbf{a}(n)) \ge m. \tag{8}$$

In Ref. [9], we proved that there exists a unique real solution of $\{\langle O_{\tilde{\mathbf{a}}(n)}^{[n]}|\ln \rho_m^{[n]}\rangle\}$ satisfying the above system of equations for a three-qubit system. This result is also valid for a general multipartite quantum state with a finite dimensional Hilbert space. Here we neglect the proof because it is a simple generalization for the three-qubit case. Thus we have two different ways to use the system of equations (7, 8). On one hand, we can use them to verify whether the solution of the optimization problem (4) is correct. On the other hand, we can directly use the optimization method to solve them to obtain the states $\rho_m^{[n]}$. In our present numerical algorithm, we adopt the latter method in application of the system of equations (7, 8). We want to emphasize that Eq. (2) is used to represent a multipartite quantum state in our algorithm.

For an optimization problem, one of the key skills is to choose a proper initial value. Here we adopt a continuity approach to choose a proper initial value for any n-partite quantum state $\rho^{[n]}$. We consider a seriers of states

$$\rho^{[n]}(p_0) = p_0 \frac{I^{[n]}}{d^{[n]}} + (1-p_0)\rho^{[n]}. \tag{9}$$

We take $p_0 = 1 - \frac{k}{N}$ with $k \in \{0, \cdots, N\}$, where N is a large positive integer. Obviously, $\rho^{[n]}(k=0) = \frac{I^{[n]}}{d^{[n]}}$, $\rho^{[n]}(k=N) = \rho^{[n]}$, and $\langle O^{[n]}_{\tilde{\mathbf{a}}(n)} | \ln \rho^{[n]}_m(k=0)\rangle = 0$. We take the values of $\{\langle O^{[n]}_{\tilde{\mathbf{a}}(n)} | \ln \rho^{[n]}_m(k)\rangle\}$ as the initial values of $\{\langle O^{[n]}_{\tilde{\mathbf{a}}(n)} | \ln \rho^{[n]}_m(k+1)\rangle\}$ for $k = 0, 1, \cdots, N-1$.

The basic idea under the above approach is based on the continuity principle, more precisely, the state $\rho^{[n]}(k+1)$ is very similar to the state $\rho^{[n]}(k)$, so the values of $\{\langle O^{[n]}_{\tilde{\mathbf{a}}(n)} | \ln \rho^{[n]}_m(k+1)\rangle\}$ is also near the values $\{\langle O^{[n]}_{\tilde{\mathbf{a}}(n)} | \ln \rho^{[n]}_m(k)\rangle\}$. The practice of our computations shows that our selection of initial values makes the algorithm become efficient. The cost of the algorithm is that we calculate the degrees of irreducible multiparty correlations for a series of states $\rho^{[n]}(p_0)$ instead of a single state $\rho^{[n]}$.

An obvious advantage is that the choose of initial values in our algorithm is independent of the state $\rho^{[n]}$. In other words, our algorithm makes the computation of a general multiparty state become efficient. In my personal computer, it is efficient for any state up to five qubits. To the best of my knowledge, it is the best results on multiparty correlations in a multiparty state we obtained so far.

Numerical results.— We will demonstrate the power of our numerical algorithm by explicitly giving the results on irreducible multiparty correlations for some typical multiparty states: the 4-qubit GHZ state [17], the four-qubit Smolin state [18], and the 5-qubit W state [19].

The first state we consider is the n-qubit GHZ state $|\mathrm{GHZ}_n\rangle = \frac{1}{\sqrt{2}}(\prod_{i=1}^n \otimes|0\rangle_i + \prod_{i=1}^n \otimes|1\rangle_i)$. The degrees of irreducible multiparty correlations on the 4-qubit GHZ state are given in Figure 1. The total correlation in the state is 4 bits, and it is classified into 3 bits of irreducible two-qubit correlation and 1 bit of irreducible four-qubit correlation. These results are the same as those given in Ref. [8], and they are consistent with the conclusion in Ref. [20, 21].

The second state we consider is the 4-qubit Smolin state, whose density matrix is simply given by $\rho^{[4]}_{\mathrm{smo}} = \frac{1}{16}(I^{[4]} + \prod_{i=1}^4 \sigma_x^{(i)} + \prod_{i=1}^4 \sigma_z^{(i)})$. We find that there exists 2 bits of correlation in the state, and they are irreducible 4-qubit correlations, which is shown in Figure 2. From the density matrix of the Smolin state, we know that it is also a generalized stabilizer state defined in Ref. [8]. In this sense, the numerical results also verify the results in Ref. [8].

The third state we consider is the 5-qubit W state $|\mathrm{W}_5\rangle = \frac{1}{\sqrt{n}} \sum_{i=1}^n \sigma_x^{(i)} \prod_{j=1}^5 \otimes|0\rangle_j$. Our numerical results show that only irreducible two-qubit correlations exist in the W state, which support the conclusion in Ref. ([22]).

In the range of our numerical results, we find that the degree of the total correlation C_T is a non-increasing

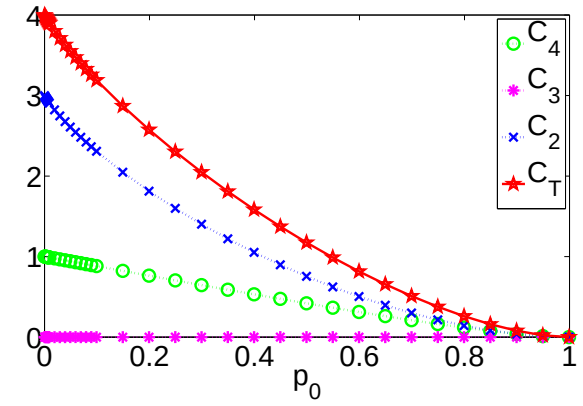

Figure 1: The degrees of irreducible multiparty correlations for the 4-qubit GHZ state.

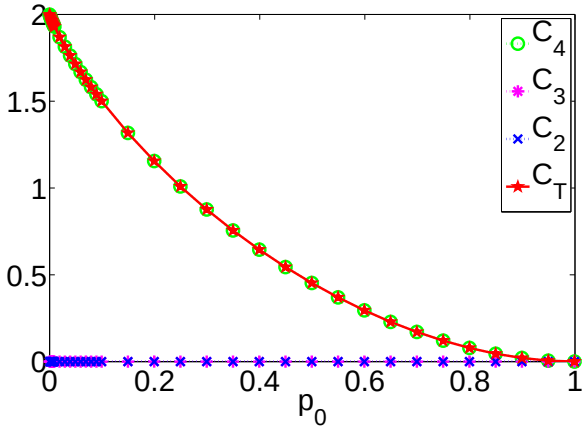

Figure 2: The degrees of irreducible multiparty correlations for the four-qubit Smolin state

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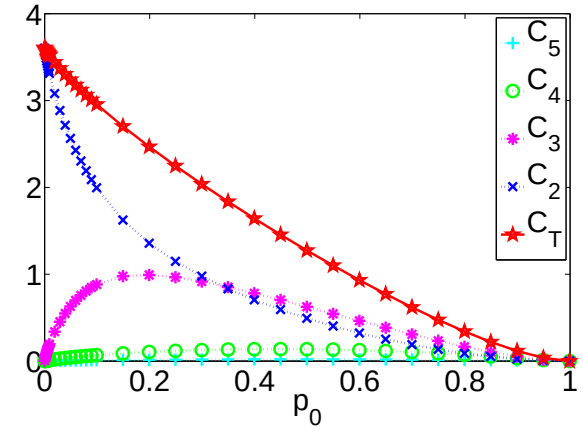

Figure 3: The degrees of irredcible multiparty correlations of the 5-qubit W state.

function of p_0, however, the degree of irreducible m-party correlation can increase with increasing p_0 (see, for example, Figure 3). Actually we can prove that $C_T(\rho^{[n]}(p_0))$ is a non-increasing function of p_0 for any n-party state $\rho^{[n]}$ as follows. We can imagine that every subsystems of the n-partite quantum system pass through a depolarized channel [23], then the quantum state $\rho^{[n]}$ evolves according to Eq. (9) in the direction of increasing p_0. In the process, only local operations act on the state $\rho^{[n]}$, and the degree of total correlation does not increase under local operations, therefore $C_T(\rho^{[n]}(p_0))$ is a non-increasing function of p_0 for any n-party state $\rho^{[n]}$.

In addition, the fact C_m $(m = 3, 4, 5)$ is not a non-increasing for a 5-qubit W state gives another example to support one of the main results in Ref. [9]: local operations can transform lower order correlations into higher order correlations.

Discussions and summary.— The calculations of the degrees of irreducible multiparty correlations for an arbitrary multiparty quantum state are challenging because they are defined as the constraint optimization problems over all the multiparty quantum states in the whole Hilbert space. In this Letter, we develop an efficient numerical method to calculate the degrees of irreducible multiparty correlations for any multipartite quantum state, which is based on the following two key elements.

One key element in our algorithm is that we adopt the expansion of a multipartite state in the exponential form (2). First, it ensures the positivity of the state automatically. Second, although the independent variables $\{\langle O^{[n]}_{\tilde{\mathbf{a}}(n)}|\ln\rho^{[n]}\rangle\}$ can take the limit to infinity, the state $\rho^{[n]}$ is always well defined because of the constraint $\mathrm{Tr}\rho^{[n]} = 1$. In this sense, the state without maximal rank are naturally contained in this expansion if the coefficients can limit to infinity. This makes our algorithm effective for arbitrary multiparty states.

The other key element is related to the selection of the initial values of variables, more precisely, the formula (9). It makes our algorithm independent on the initial values of variables, and greatly enhances the efficiency of our algorithm.

In summary, we present an efficient numerical algorithm on the calculations of the degrees of irreducible multiparty correlations in a multiparty quantum state. Our algorithm is valid for arbitrary quantum states up to five qubits in my personal computer, and it is a universal algorithm whose efficiency does not depend strongly on the multipartite quantum state. We demonstrate the power of our algorithm by explicitly giving the results for the 4-qubit GHZ state, the Smolin state, and the 5-qubit W state, which are consistent with previous results. We hope that our development of this algorithm will provide a powerful tool to analyze the correlation distributions in a multipartite quantum state, and thus takes a crucial step towards the practical applications of irreducible multiparty correlations in real quantum many-body systems.

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